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Multi-Physics Demonstration Problem with the SHARP Reactor Simulation Toolkit: LLNL Contribution

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Auspices

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Prologue

In FY14, a joint team from Argonne National Laboratory (ANL) and Lawrence Livermore National Laboratory (LLNL) performed a joint study under the DOE-NE Advanced Reactor Concepts (ARC) program. This comprised the specification of a full-core fast reactor simulation demonstration and its subsequent execution with the SHARP toolkit. SHARP combines neutronic, thermal-fluid and structural mechanics codes via a flexible data backplane. The Diablo code [1] provides the structural mechanics functionalities for SHARP. The successful completion of the milestone calculations was documented in an integrated report published by ANL [2], fulfilling their deliverable under milestone M2AR-14AN1701088. This present document records the text and figures drafted by the LLNL contributors to that report. Final edits were controlled by ANL and thus its integrated report should be consulted for final results.

Section 5.3. Standalone DIABLO Solid Mechanics Simulations

The mulitphysics (Solid Mechanics, Heat Transfer, Advection/Diffusion, and Electromagnetics) code DIABLO is here used only for Solid Mechanics calculations, e.g., temperature data provided by Nek5000 is used to predict the resulting deformations. DIABLO requires the following inputs: The "mesh" file providing spatial definitions, here communicated as either an EXODUS or future MOAB file; an assembly file containing global data such as material and friction model information, time step, solution algorithm-related controls (convergence criteria, linear solver, nonlinear iteration technique), and input/output related controls (restart, plotting, coupling to external codes/data); and a "subassembly" file which maps specific spatial quantities in the mesh description (nodesets, sidesets, element blocks) to Diablo element sets incorporating material model assignment, interface contact sets, and boundary conditions. The "subassembly" file also contains controls for individual element and contact sets, such as integration method, penalty stiffness scaling, etc. The collective problem definition is illustrated in Figure 5.c.1.

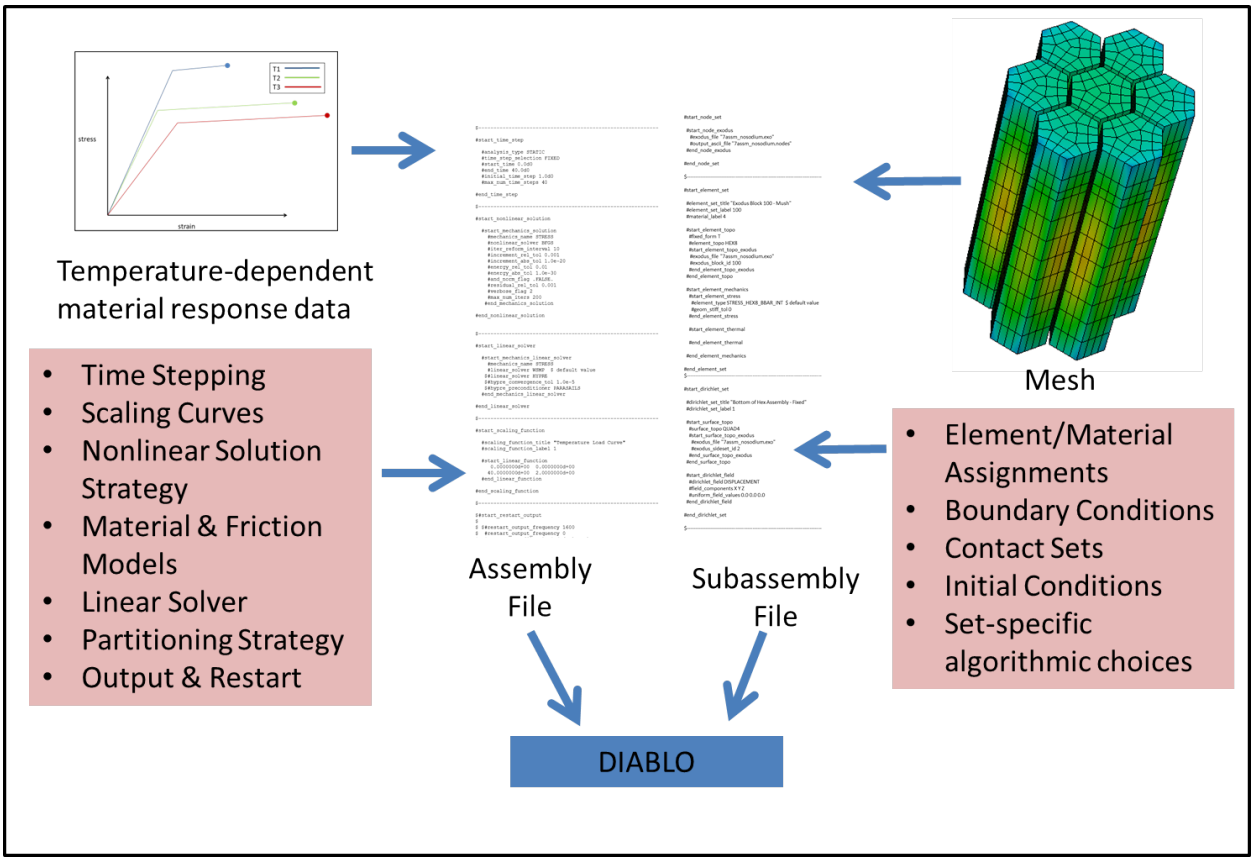

Figure 5.c.1. Problem definition required by DIABLO.

The mesh for each case (seven assembly and full core) was described in a previous section, but we again emphasize here that the assembly ducts, load pads, restraint ring, and inter-assembly sodium gap are represented explicitly (heterogeneously) in the geometry. The assemblies themselves (interior of the duct) were fully homogenized. The geometry was coarsely meshed with linear finite elements in order

to keep the number of degrees of freedom reasonably small for the full-core case which has to fit on ANL's Cosmea platform (128 processors).

In the ultimate vision, DIABLO will only require a subset of the overall domain, the Structural Components. These are

- Structural Components:
    - Duct Wall
    - Homogenized Duct Interior
    - Load Pads
    - Restraint Rings

In contrast, NEK and PROTEUS consider a different subset of the domain, the HydroNeutronic Components

- HydroNeutronic Components
    - Duct Wall
    - Homogenized Duct Interior
    - Upper Sodium
    - Outer Sodium (including load pad and restraint rings modeled as sodium fill)

Only some of the components are common to the Structural Mechanics and the HydroNeutronics:

- Common Components
    - Duct Wall
    - Homogenized Duct Interior

The result of the simulation of the Structural Components will be used to construct a smooth displacement field throughout the NEK and PROTEUS simulation domains. This will be accomplished by using a mesh smoothing capability of the MOAB framework to construct a deformed mesh for the HydroNeutronic Components (NEK and PROTEUS meshes) from the displacements calculated by DIABLO on the Common Components. Note that the Common Components do not include the Load Pads and the Restraint Rings as modeled by DIABLO, since it is assumed they will contact during the simulation, and the resulting "zero-thickness" elements in the gap between them would not be admissible in a NEK or PROTEUS simulation.

As a risk mitigation during development of the MOAB smoothing machinery, DIABLO is currently being run to directly compute all required deformations for the HydroNeutronic Components. This requires using Duplicated Components in select, limited regions, i.e., certain elements and nodes have been duplicated in space and modeled as two different materials. This allows DIABLO to compute a valid deformed mesh for the HydroNeutronic Components while at the same time correctly taking into account mechanical contact between load pads and between load pads and the restraint rings.

- Duplicated Components
    - Load Pads and Restraint Rings

Hence, a Composite Mesh is used to compute deformations and a smooth mesh redistribution across the entire computational domain:

- Composite Mesh:
  - Duct Wall
  - Homogenized Duct Interior
  - Load Pads, with mechanical contact
  - Restraint Rings, with mechanical contact
  - Upper Sodium
  - External Sodium
  - Load Pads (duplicated), modeled as External Sodium
  - Restraint rings (duplicated), modeled as External Sodium

Only a subset of the Composite Mesh is communicated to NEK and PROTEUS, consisting of

- Composite Mesh communicated to NEK and PROTEUS:
  - Duct Wall
  - Homogenized Duct Interior
  - Upper Sodium
  - External Sodium
  - Load Pads (duplicated), modeled as External Sodium
  - Restraint Rings (duplicated), modeled as External Sodium

At this stage, very simple structural material models are being used. The duct walls, restraint rings, and load pads are all modeled as linearly elastic stainless steel. DIABLO Material Model 4 (Finite deformation elastic/plastic with temperature-dependent properties) is being utilized, but for simplicity as we begin to explore the simulation space we have begun by using this model in the purely elastic, temperature-independent model. The Homogenized Duct Interior, External Sodium, and Upper Sodium are modeled as very soft linear elastic material.

Table 1. 9-Material Properties.

Material	Density g/cc	Young's Modulus Dyne/cm^2	Poisson's Ratio	Thermal Expansion Coefficient
Duct Wall (SS)	1.746E+04	1.93E+10	0.29	1.227E-5
Load Pad (SS)	1.746E+04	1.93E+10	0.29	1.227E-5
Restraint Ring (SS)	1.746E+04	1.93E+10	0.29	1.227E-5
Homogenized Interior	1.746E+04	1.93E+4	0.29	1.227E-5
External+Upper Sodium	1.746E+04	1.93E+4	0.29	1.227E-5

Boundary conditions, initial conditions, and contact definitions are required to complete the analysis. In the actual structure, a complicated socket/nozzle arrangement exists at the base of each assembly. This allows for a limited amount of hex can rotation to occur at the base before contact occurs with the socket, constraining subsequent rotation. The details of this joint are highly dependent on manufacturing tolerances, can and socket aging/swell, and refueling insertion force. For this first demonstration it was decided to use the following boundary condition:

- Baseline Boundary Condition
    - Duct Walls and Duct Homogenized Interior Fixed (ux=uy=uz=0) at Z=Zmin

It was found for the Composite Mesh that no boundary condition was required for the restraint rings – they float up and down vertically as forced by the thermal expansion of the outer sodium, which keeps them lined up in the axial direction with the load pads, and they are strong enough in the hoop direction to withstand expansion forces caused by contact between the rings and the duct walls. Future work may include direct modeling of the surrounding core barrel to which the restraint rings are attached.

- Baseline Initial Condition
    - Initial Temperature = 300K (uniform across the mesh)

The first chosen initial condition is representative of the actual deformation of the structure. Choosing an initial temperature closer to the average operational temperature (a value of 550K has been suggested) would result in a smaller perturbation to the initial mesh. Ultimately, if convergence of the multi-physics coupled solution becomes a problem, under-relaxation techniques may be applied to the deformation (the output of the solid mechanics simulation) to allow the coupled system to smoothly approach convergence.

A mortar contact algorithm is used where each load pad, as a “slave”, is restrained from penetrating the surrounding load pads and the restraint rings. Two contact sets per duct assembly are therefore required (14 contact sets for the 7 assembly model and 398 for the 199 assembly model). Currently a penalty/augmented Lagrange algorithm with a tolerance of 1.0e-2 on the total interface contact force is being used, and frictionless contact is assumed. Future work will include investigation of the influence of friction, but as the interface is filled with liquid sodium it is assumed the effect of friction is small.

Standalone structural deformation calculations are possible, using temperatures either from Nek/Proteus bi-physics simulation or through the construction of synthetic temperature fields. For the 7 assembly models, preliminary temperature distributions were available from coupled PROTEUS/NEK runs with the undeformed geometry, and these will be used for the “standalone” demonstration. For the full core model, PROTEUX/NEK runs were not yet available and the deformation was driven by a synthetic temperature field.

Section 5.a.i. Seven Assembly Core (Three Fuel Assemblies)

The first seven-assembly problem is a mini-core comprised of seven assemblies taken from the ABTR design. Three fuel assemblies, two reflectors, one shield, and one control assembly are arranged in the

configuration (2D view) shown in Figure 2. The three fuel assemblies were assigned the “inner core” fuel composition. Note the duct and inter-duct sodium gap are represented explicitly.

We emphasize that this small test case was formulated to test each of the assembly types (i.e. ensuring that the mesh could be imported and used by each of the physics codes) as well as the restraint ring geometry and the “composite model” techniques of node/element duplication. It does not represent a realistic reactor core. The case uses the minimum number of total assemblies to test all four assembly types in hexagonal geometry. Keeping the problem size small allows for less cumbersome debugging and input preparation.

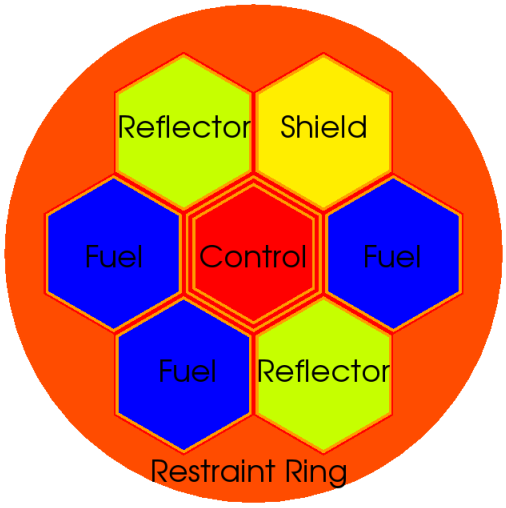

Figure 2. Seven assembly core configuration containing three fuel assemblies.

Figure 3 depicts the mesh for this problem; the seven assemblies and restraint ring region can easily be seen. The thick black lines are actually the outline of the duct wall and inter-assembly sodium gap. This mesh consisted of 25,776 elements and 27,625 vertices, which is relatively small for DIABLO and can easily be run in serial mode. When running with the composite geometry (with the load pads and constraint rings duplicated along with certain of their nodes), there are 26,264 elements and 28,685 vertices. Figure 4 shows the model stripped of the outer sodium (material model 8) and the duplicated elements/nodes. Regions defined as Material 1 represent the duct wall. Material 2 is the region of the upper (TLP) restraint ring, here modeled as outer sodium. Material 3 is the region of the upper (TLP) load pads, here modeled as outer sodium. Material 4 is the lower (ACLP) restraint ring, here modeled as outer sodium. Material 5 is the region of the lower (ACLP) load pads, here modeled as outer sodium. Material 6 is the homogenized duct interior (not seen in the picture), and Material 7 is the upper sodium. Figure 5 shows the structural restraint system: Material 9 is the upper (TLP) load pad modeled as stainless steel, Material 10 is the lower (ACLP) load pad, modeled as stainless steel, Material 11 is the lower (ACLP) restraint ring, modeled as stainless steel, and Material 12 is the upper (TLP) restraint ring, again modeled as stainless steel.

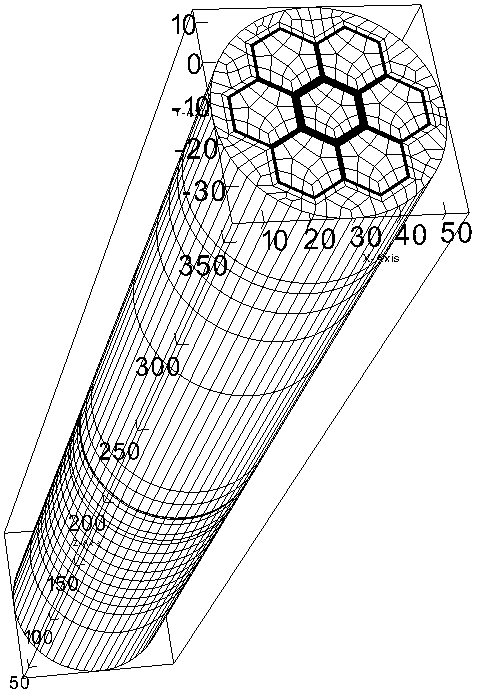

Figure 3. Mesh view of seven assembly case with three fuel assemblies.

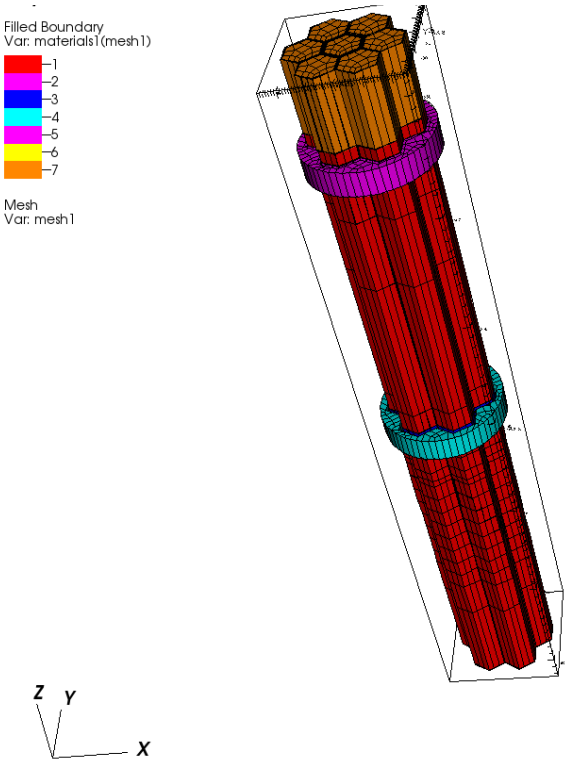

Figure 4. 3D View of Restraint Rings, Hex Cans, and Upper Sodium with External Sodium removed

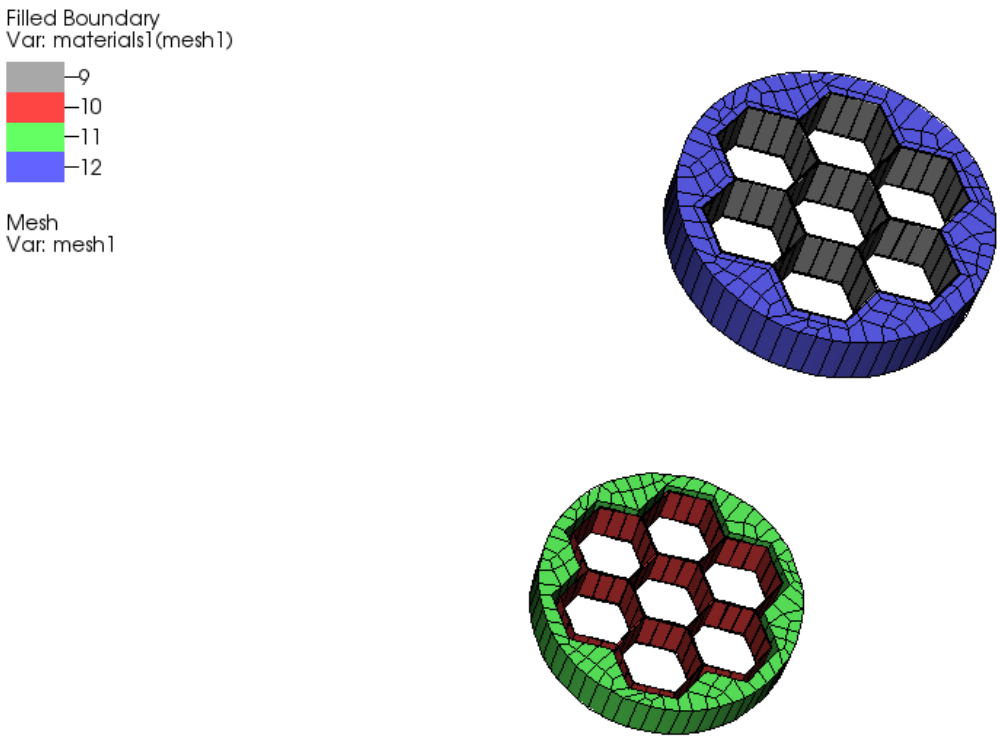

Figure 5. Restraint Rings and Load Pads.

Figure 6 shows the temperature distribution loaded from the initial NEK/PROTEUS run. Note that most of the elevated temperature is in the central control assembly. The maximum temperature over the entire mesh is 641 K and the minimum is 594 K, a range of only a little over 40 K. The initial temperature for the DIABLO run was set to 400K. Figure 7 shows an example of the deformed geometry, superimposed over a wireframe version of the undeformed mesh.

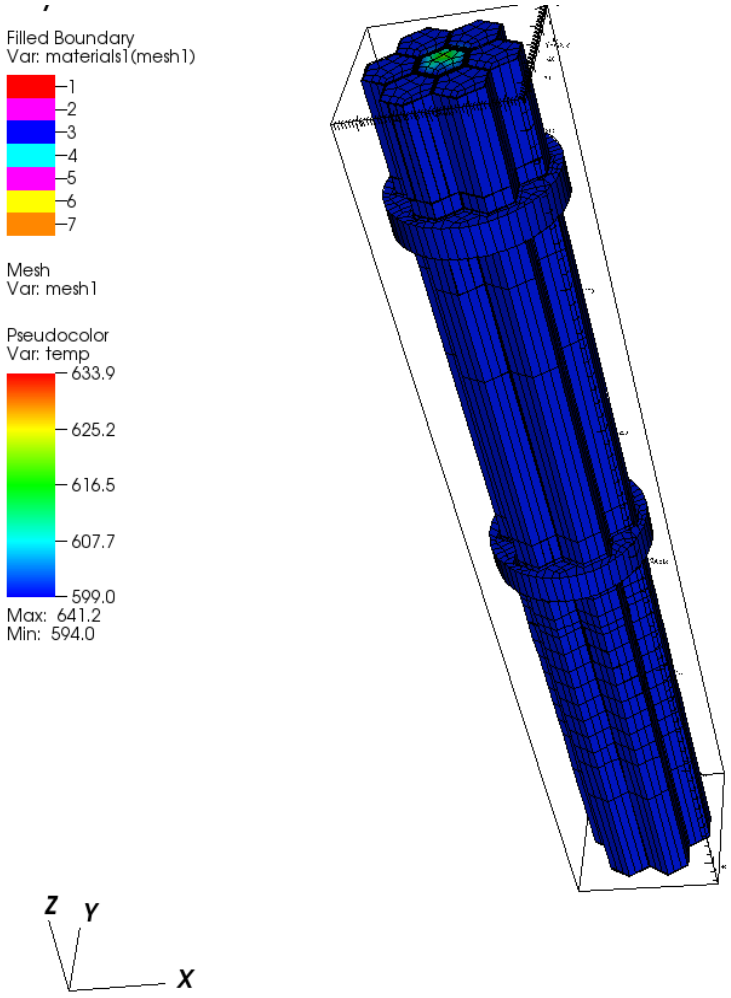

Figure 6. Temperature distribution from initial NEK/PROTEUS run

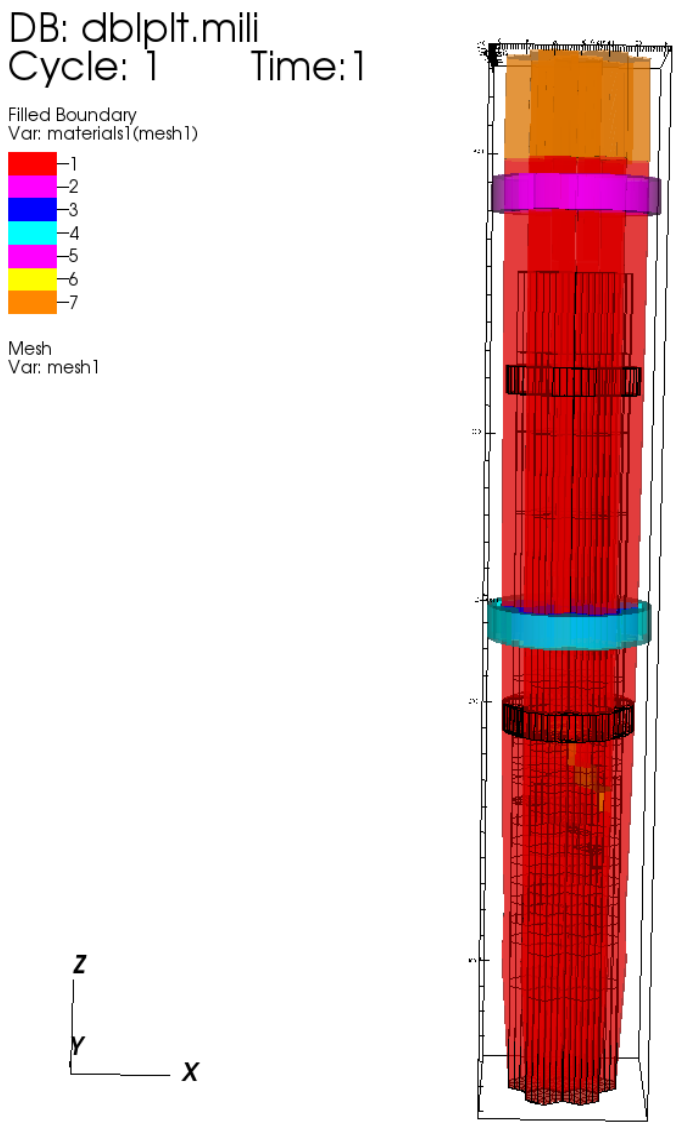

Figure 7. Deformed Geometry superimposed over undeformed mesh in wireframe. Displacements exaggerated by a factor of 100

Section 5.a.ii. Seven-Assembly Core (Seven Fuel Assemblies)

Due to the limited amount of fuel and unrealistically asymmetric power distribution in the previous test case, a second small test problem was defined with seven fuel assemblies (again using inner core fuel). The core map is shown in Figure 8.

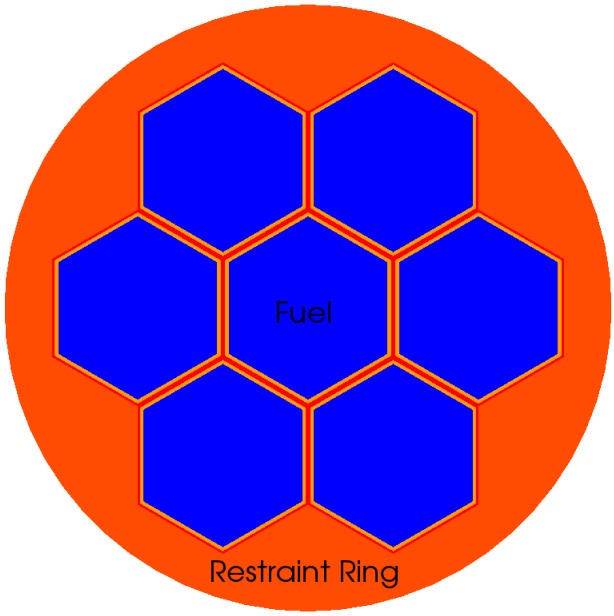

Figure 8. Composition map for 7-assembly core with 7 fuel assemblies.

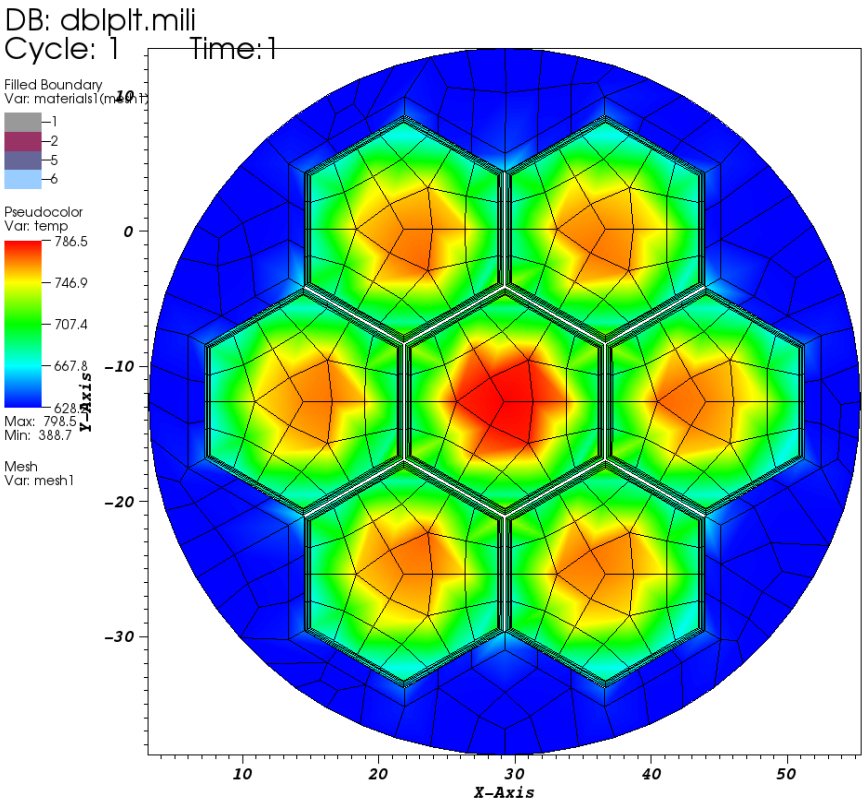

Figure 9. Temperature Distribution in the All Fuel Mesh

The displacements for this mesh were also computed.

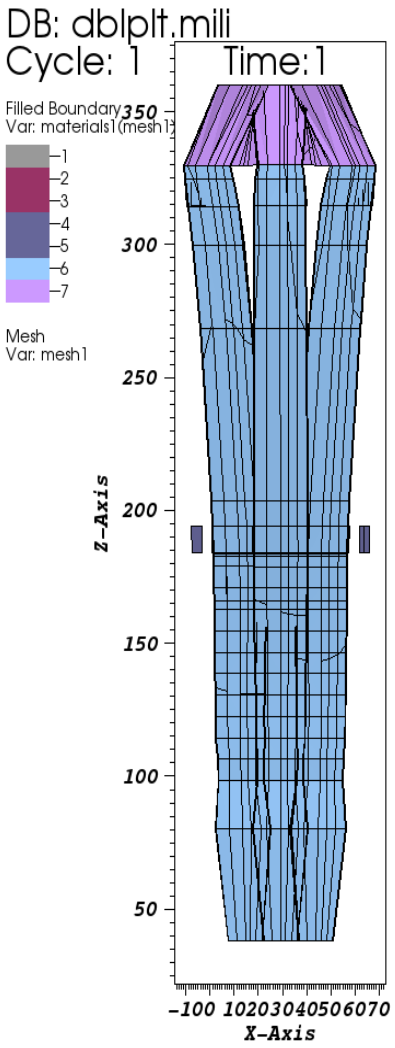

Figure 10. Displaced Mesh, scaled by a factor of 100.

Section 5.a.iii. Full Core Problem

The full core ABTR problem has 199 assemblies in total, including 60 fuel assemblies. The total power is set to 250 MWt based on the specification. The fuel assemblies are comprised of three different types: inner core, outer core, and fuel test assemblies which differ only by fuel composition. The core map is shown below. Note the explicit representation of the double duct in the control assemblies.

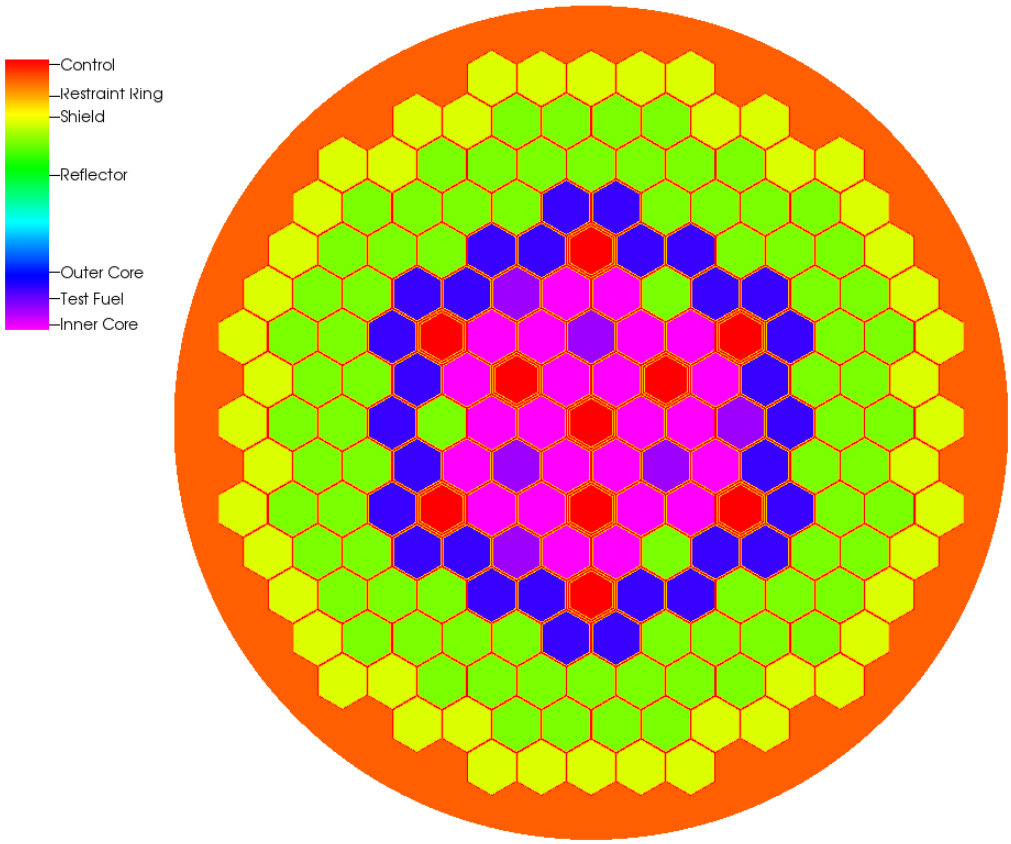

Figure 11. Full Core Composition Map Showing Explicit Ducts.

The full core mesh has 825,125 vertices and 789,696 elements. As in the 7 Assy Case, duplicate nodes/elements result in a slightly larger problem size when running the Composite Model. Parallelization is necessary in order to reduce memory per processor requirements as well as the computer wall-clock time. DIABLO is highly parallelizable, and 32 processors were used to run the full-core problem based on availability of the Cosmea cluster. The total wall-clock time using 64 processors was less than 15 minutes for the standalone calculation. When contact interfaces become active, the problem becomes much more computationally intensive, and it is expected that 64-128 processors will be necessary to keep the simulation time down to less than an hour.

Figure 13, 14, and 15 shows the mesh with material assignments from three vantage points. We calculated a deformed configuration for a test case of this mesh, using a synthetic temperature profile, which is illustrated in Figure 16. Figure 17 shows the deformed configuration, scaled by a factor of 100, with the temperature profile laid on top.

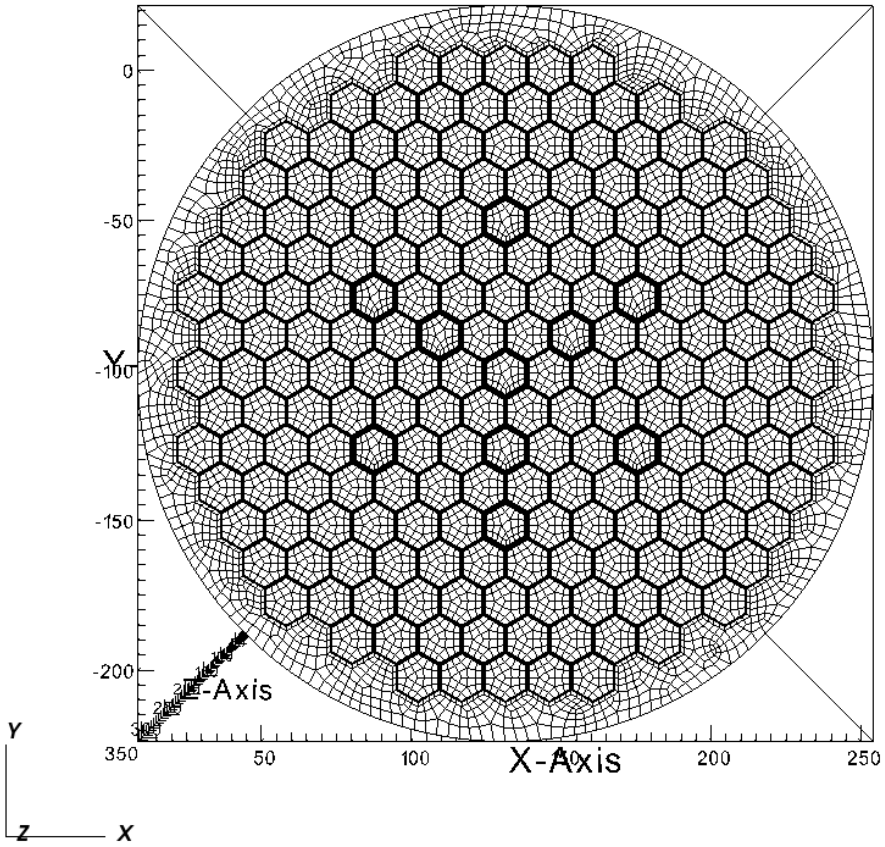

Figure 12. Top View of Full Core Mesh.

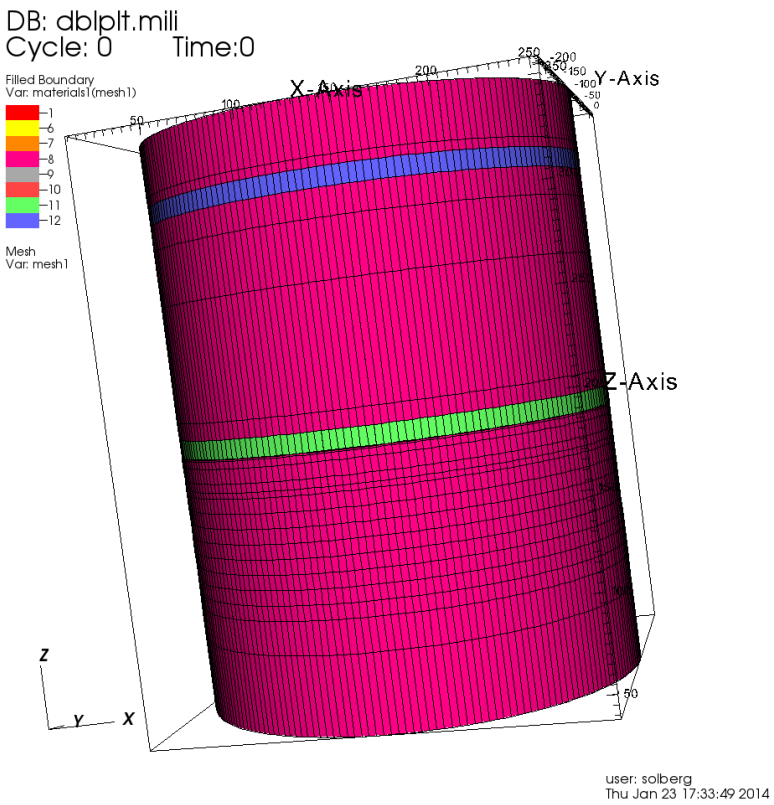

Figure 13. Full Core Mesh side view

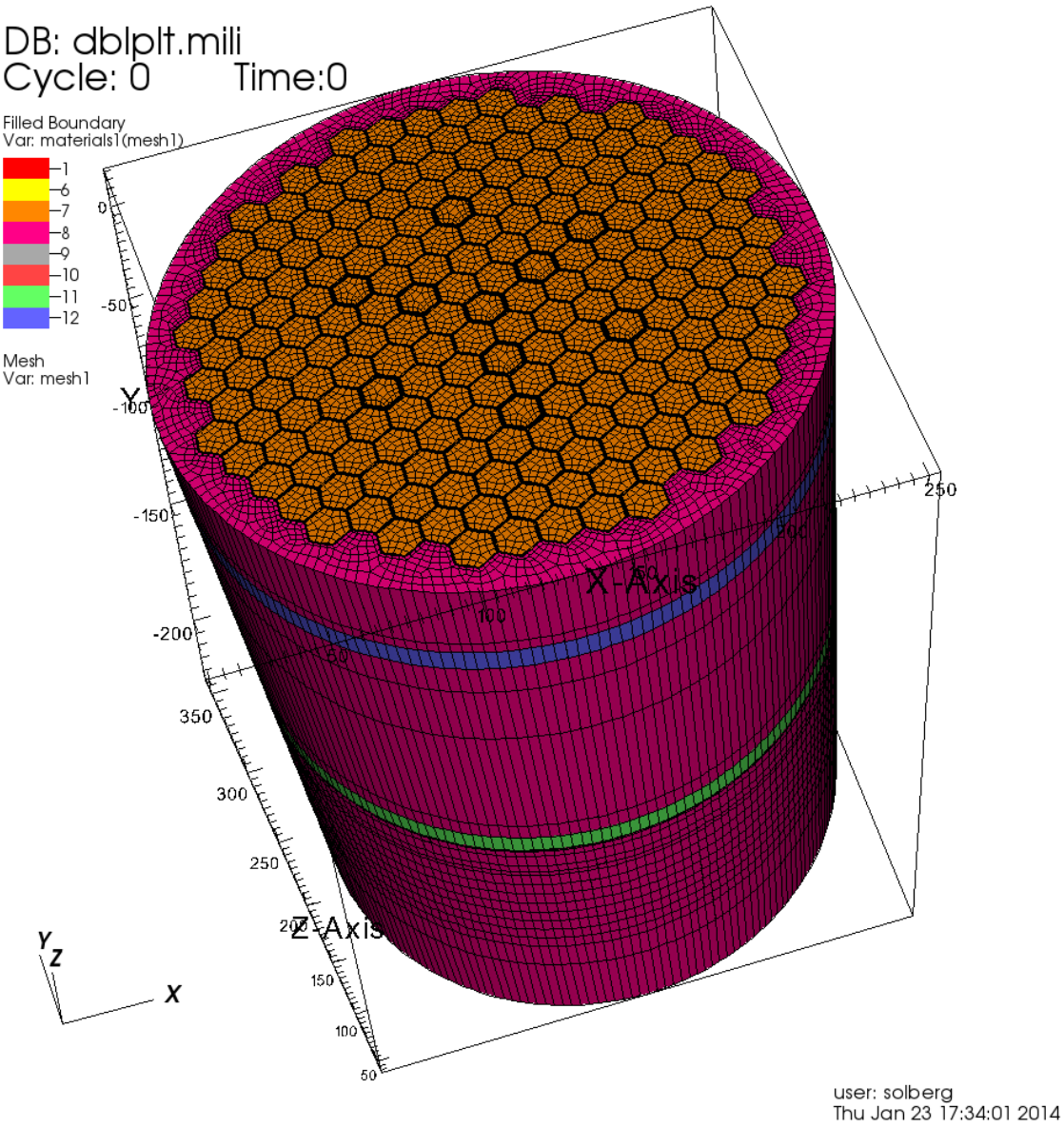

Figure 14. Mesh, top view.

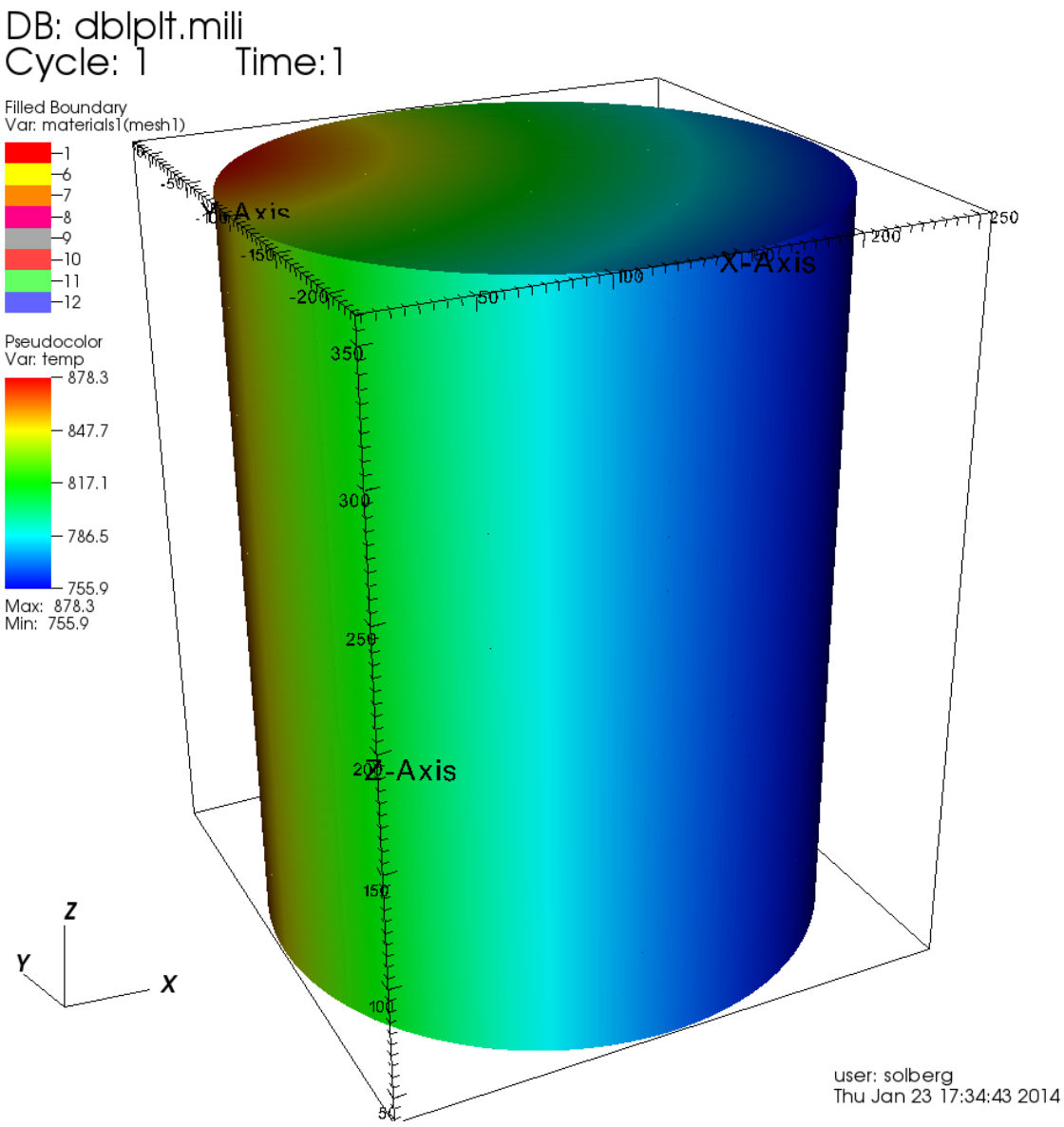

Figure 15. Synthetic Temperature Distribution

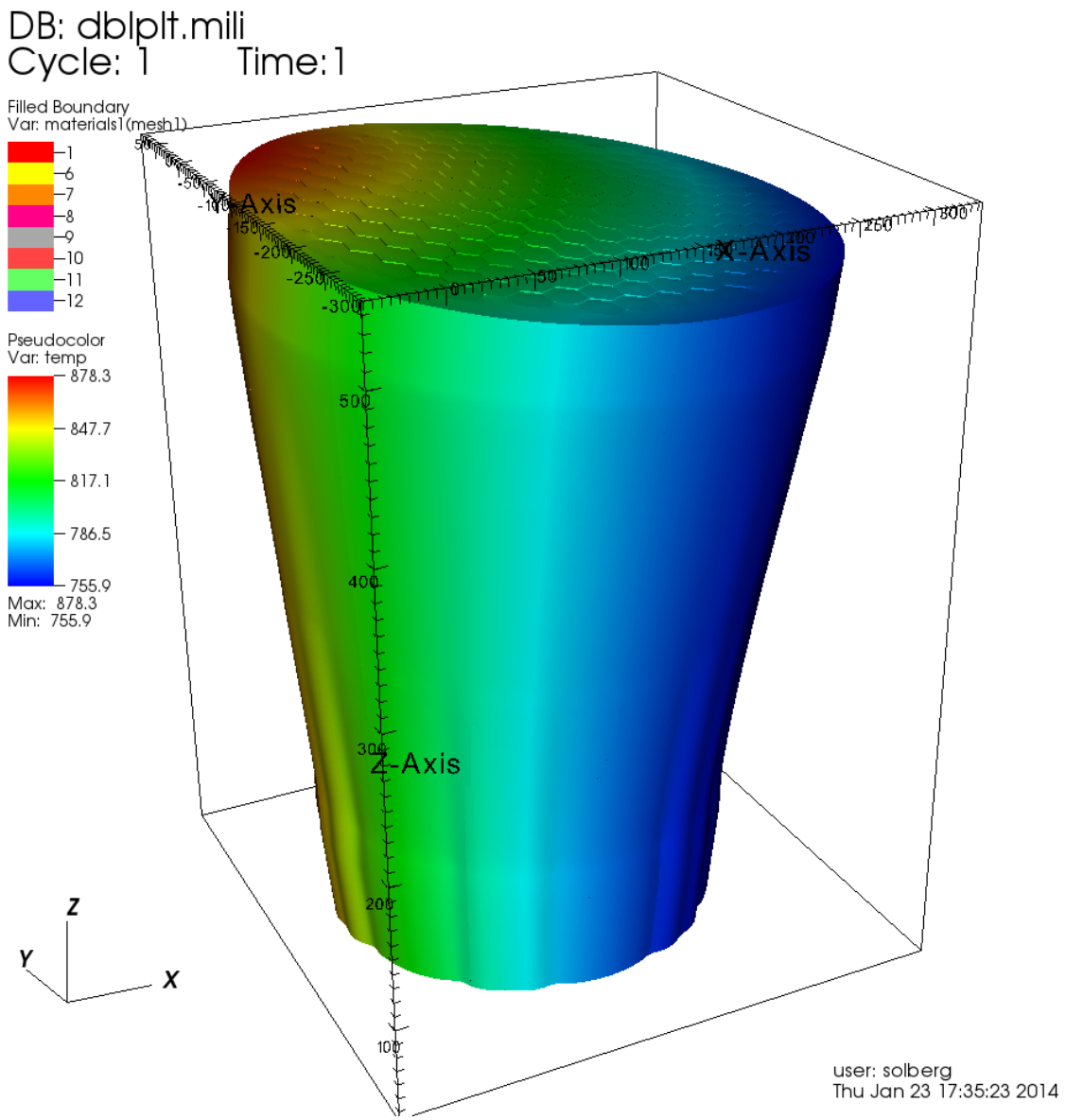

Figure 16. Displacements due to Synthetic Temperature Distribution, Scaled by a factor of 100

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[1] Solberg, J. M., Hodge, N. E., Ferencz, R. M., Parsons, I. D., Puso, M. A., Havstad, M. A., *et al.* (2014). Diablo: A parallel multi-physics finite element code for engineering analysis User Manual, v3.0. Lawrence Livermore National Laboratory, Methods Development Group, LLNL-SM-651163.

[2] E. Merzari, E. Shemon, J.W. Thomas, A. Obabko, R. Jain, V. Mahadevan, T. Tautges, J. Solberg, R. Ferencz, R. Whitesides, "Multi-Physics Demonstration Problem with the SHARP Reactor Simulation Toolkit", Argonne National Laboratory, ANL-ARC-284, 2014.